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An ASABE Meeting Presentation

Paper Number: 085112

AnnAGNPS Application and Evaluation in NE Indiana

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**Written for presentation at the
2008 ASABE Annual International Meeting
Sponsored by ASABE
Rhode Island Convention Center
Providence, Rhode Island
June 29 – July 2, 2008**

Abstract. The Annualized Agricultural Non-Point Source (AnnAGNPS) pollution model was developed for simulation of runoff, sediment, nutrient, and pesticide losses from ungaged agricultural watersheds. Here, the model was applied to the 707 km² Cedar Creek Watershed (CCW) and the 45 km² Matson Ditch Sub-Catchment (MDS), which are predominantly (>85%) agricultural, with major crops of corn and soybeans. Atrazine herbicide is of significant concern, as the St. Joseph River is the source of drinking water for the city of Fort Wayne, Indiana. Major objectives were to evaluate the ability of AnnAGNPS to simulate runoff and atrazine concentrations in uncalibrated, calibrated, and validation modes. Data sources for the model inputs included USGS Digital Elevation Model for topography, NRCS spatial SSURGO soils data, and the USDA-NASS cropland data layer. Observed flow data for CCW were available from a USGS gaging station, while flow and atrazine concentration data were available from a NSERL water quality sampling site at the discharge point of the MDS. In an uncalibrated mode, flow discharge predictions by AnnAGNPS were satisfactory at the CCW scale, but could be improved through calibration. Flow discharge for both CCW and MDS could be well matched with observed during model calibration, as could discharge for CCW during model validation. Initial AnnAGNPS predictions of atrazine concentrations in runoff water were very poor, and it was impossible to improve the results through any type of calibration. Inspection of the model source code revealed a unit conversion error in the runoff value being utilized in the pesticide routine, which when corrected greatly improved the results. The corrected AnnAGNPS model code could be successfully calibrated and validated for predictions of atrazine concentrations in the MDS.

Keywords. Watershed, modeling, non-point source pollution, runoff, atrazine

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AnnAGNPS Application and Evaluation in NE Indiana

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Introduction

Agriculture and its impacts on the environment are becoming increasingly important. During the past five years, assessment of the effects of soil conservation practices on water quality have been under study by a large group of scientists in the USDA-Agricultural Research Service (ARS). This Conservation Effects Assessment Project (CEAP) is aimed at determining what benefits are seen in (initially) water quality in a number of watersheds across the United States (Mausbach and Dedrick, 2004).

The ARS CEAP is divided into 5 components: 1.) Develop/implement a database system for collection and dissemination of information from the watershed studies; 2) Measure water flow and quality and determine the impacts of conservation practices on water quality at the watershed scale across a range of agricultural and environmental conditions; 3) Apply water quality models to determine their effectiveness in simulating the effects of various conservation practices on water quality; 4) Conduct economic analyses and develop tools to assist in selection and placement of conservation practices to optimize profits as well as environmental benefits; and 5) Develop new regional water quality models to better assess the impacts of conservation practices in major agricultural regions.

One of the fourteen ARS Benchmark Watersheds for CEAP is the St. Joseph River Watershed in northeastern Indiana (with parts in northwestern Ohio and southern Michigan). This 281,000 ha basin is predominantly agricultural land (79%), with 10% in woodlands/wetlands, and the remaining 11% in a variety of land uses (urban, farmstead, industrial, etc.). The St. Joseph River is the source of drinking water for the city of Ft. Wayne (population ~250,000). Recent research activities in the watershed have focused on monitoring of runoff waters in ditches and streams to identify nutrient and pesticide contaminants, modeling of runoff and pollutant transport, and development of management practices to reduce pollutant losses to the river (Flanagan et al., 2008).

This paper deals with activity under CEAP component 3, in regards to applying water quality models to determine their applicability and performance. The two models identified for use in CEAP are the Soil and Water Assessment Tool (SWAT, Arnold et al., 1998) and the Annualized AGricultural Non-Point Source pollution model (AnnAGNPS, Bingner and Theurer, 2005). Other researchers at Purdue University and the USDA-ARS National Soil Erosion Research Laboratory (NSERL) have examined the applicability and performance of SWAT (Vazquez-Amabile et al., 2006; Larose et al., 2007) in the St. Joseph River Watershed and its subwatersheds. The objective of this study was to apply and evaluate the AnnAGNPS model there.

This paper will describe the AnnAGNPS modeling study, the datasets used, uncalibrated model results, and calibrated/validated model results. Additionally, an error present in the AnnAGNPS code will be described and the correction necessary identified to allow for much improved simulation of pesticide transport.

Background

The largest tributary to the St. Joseph River is Cedar Creek, draining about 707 km² with drainage areas in DeKalb, Allen, and Noble Counties, Indiana (Figure 1). The Cedar Creek Watershed (CCW) is located in the northeast Indiana portion (41°04'48" to 41°56'24" N and 84°52'12" to 85°19'48"W) of the St. Joseph River Watershed. CCW is comprised of two 11-digit hydrologic unit code watersheds, the Upper (04100003080) and Lower Cedar Creek (04100003090). The Matson Ditch Sub-catchment (MDS) of the CCW, located within DeKalb County, Indiana, drains approximately 45 km² of predominantly agricultural land in the northeast portion of the CCW (Figure 1). The topography of the CCW is generally flat to gently rolling with morainal hills composed of till or sand and gravel with local relief ranging from 30 to 60 meters and many depressional areas that hold water after large rainfall events (SJRWI, 2005; Greeman, 1994). The CCW has an elevation minimum of 238.31 m and maximum of 326.25 m above sea level with the lowest point located in Allen County near the confluence of Cedar Creek and Matson Ditch.

Orientation of Cedar Creek Watershed and Matson Ditch Sub-catchment

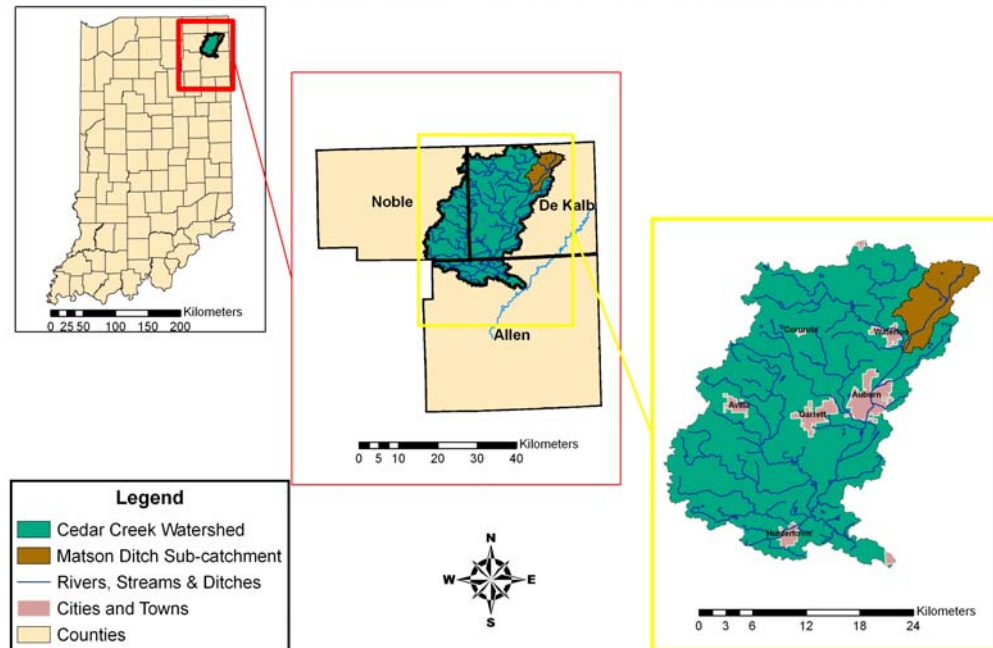


Figure 1. Cedar Creek Watershed in Northeast Indiana.

Previous water quality modeling conducted in CCW with the SWAT model has been reported by Larose, 2005, and Larose et al., 2007. Larose (2005) calibrated and validated the SWAT model on daily and monthly hydrology and pesticide concentrations to assess the probability of exceeding the U.S. EPA drinking water standards. The calibrated SWAT model performed well at prediction of both hydrology and atrazine pesticide loadings.

The Annualized Agricultural Nonpoint Source Pollution model (Theurer and Cronshey, 1998; Bingner and Theurer, 2005; USDA-ARS, 2006) was developed by the USDA Agricultural Research Service (ARS) and Natural Resources Conservation Service (NRCS) to predict sediment and chemical delivery from ungaged agricultural watersheds up to 300,000 ha (Bosch et al., 2001). AnnAGNPS is a continuous simulation, grid-based, batch-process computer program where runoff, sediment, nutrients and pesticides are routed from their origins in upland grid cells through a channel network to the outlet of the watershed (Bingner and Theurer, 2005). The climatic data requirements for simulations include daily maximum and minimum temperature, precipitation, average daily dew point temperature and wind speed, and sky cover (Bingner and Theurer, 2005). The ArcView interface for AnnAGNPS incorporates the Generation of weather Elements for Multiple applications (GEM) climate generation model (USDA-ARS, 2005) which generates daily precipitation, maximum and minimum temperature, and solar radiation. AnnAGNPS users also have the option to input measured climate data by uploading the data into the input editor.

AnnAGNPS hydrology is based on a simple bookkeeping of inputs and outputs of water during the daily time steps (Bingner and Theurer, 2005). The hydrologic processes simulated in the model include interception evaporation, surface runoff, and evapotranspiration, subsurface lateral flow and subsurface drainage (Yuan et al., 2006). In AnnAGNPS, runoff is predicted using the SCS curve number technique (USDA-SCS, 1986), and sheet and rill erosion is predicted with the Revised Universal Soil Loss Equation (RUSLE, Renard et al., 1997). Soil moisture balance is calculated on a sub-daily time step using a simple constant-time step procedure for both the tillage and below tillage composite soil layers (Bingner and Theurer, 2005). Sediment transport in channels is computed using a modified Einstein equation, and the Bagnold (1966) equation is used to estimate sediment transport capacity of the flow (Bingner and Theurer, 2005). AnnAGNPS utilizes the HUSLE (Hydro-geomorphic Universal Soil Loss Equation) model (Theurer and Clarke, 1991) to determine sediment delivery ratios of total sediment to the stream network.

In every grid cell, a daily mass balance is used to estimate the amounts of organic carbon, nitrogen and phosphorus in soluble and adsorbed forms in the soil, applied as fertilizer or manure, as well as components in plants and residues. A pesticide mass balance in each cell is also performed each day of simulation, and accounts for materials applied to a field, foliage wash-off, transport in the soil profile, degradation, and soluble and sediment adsorbed material that moves in surface runoff (Bosch et al., 2001; Bingner and Theurer, 2005). AnnAGNPS utilizes a modified version of the Groundwater Loading Effects of Agriculture Management Systems (GLEAMS) (Leonard et al., 1987) to simulate pesticides that are attached to clay particles and those in solution. GLEAMS is a daily time step model that calculates pesticide degradation, extraction into runoff, vertical flux, transport with sediment, evaporation, and plant uptake (Leonard et al., 1987).

The AnnAGNPS model has had moderate use, mainly by researchers in the United States and Canada. Tagert (2006) performed AnnAGNPS simulations in the 13,200 ha Upper Pearl River Basin to validate pesticide loading of atrazine and metolachlor against measured grab sample data. Her event-based results showed an R^2 of 0.0954 for atrazine and 0.0616 for metolachlor when comparing measured and simulated concentrations. Suttles et al. (2003) conducted simulations with AnnAGNPS in the 333 km² Little River Research Watershed in south central Georgia, and found that average annual runoff, sediment, and nutrient loads were all under-predicted in the upper part of the watershed. In the lower part of the watershed, predicted runoff was close to the observed, but sediment and nutrients were overestimated. Yuan et al. (2003) described application of AnnAGNPS to the Deep Hollow watershed in Mississippi to evaluate nitrogen loadings, and reported poor predictions of monthly values.

Yuan et al. (2006) described enhancements to the AnnAGNPS model for simulation of subsurface flows and subsurface drainage, and presented results of the model application to the Ohio Upper Auglaize watershed, though validation was not possible due to use of only simulated climate. In Ontario, Das et al. (2007) compared the performance of SWAT and AnnAGNPS for prediction of runoff and sediment loss from the Canagagigue Creek watershed. AnnAGNPS was applied in a calibration and validation procedure, and had Nash-Sutcliffe (1970) model efficiency values of 0.79 and 0.69 for monthly runoff predictions in the calibration and validation phases, respectively. For monthly sediment losses, model efficiency values for AnnAGNPS were 0.53 and 0.35 for the calibration and validation periods, respectively.

Materials and Methods

Topography of the CCW and MDS were determined using a Digital Elevation Model (DEM) obtained from USGS at a resolution of 1/3 arc-second with an elevation resolution of ± 7 m to delineate the sub-watershed slopes, stream network, and the watershed and sub-watershed boundaries. The DEM was projected to Universal Transverse Mercator (UTM) NAD83, Zone 16 for the state of Indiana, re-sampled to an exact 10 meter grid, and burned in one meter with the stream networks from the National Hydrography Dataset (NHD). The CCW was delineated using the TopAGNPS program (Garbrecht and Martz, 1999) within the AnnAGNPS ArcView interface version 3.57 a2 (USDA-ARS, 2006) with a critical source area (CSA) of 100 ha and minimum source channel length of 100 m. This CCW delineation resulted in a total area of 703.2 km² divided into 942 cells with an average area of about 75 ha. The MDS was included in this delineation with an outlet identified at the downstream end of reach 328 with a total area of 44.7 km². This CCW delineation (703.2 km²) corresponded well with that of the USGS which identified CCW as 707.5 km² and MDS (44.7 km²) corresponded well to Hogart (1975) which identified MDS as 45.07 km².

Spatial distribution of soils for AnnAGNPS cells in the CCW and MDS (see Zuercher, 2007) were determined using the SSURGO spatial dataset. Forty-five soil SSURGO series were present in the CCW with Blount being dominant (25% of the watershed), following by Morley (16%), Pewamo (16%), and Glynwood (10%). Soil properties for the representative soils were retrieved in an AnnAGNPS input format using the National Soil Information System (NASIS) soil database. Due to a lack of soil data for muck soils and problems with how AnnAGNPS handles water cells, any AnnAGNPS cells that were determined to have predominately muck soils were converted to Blount silt loam (BaB2), the predominate soil in the watershed.

Table 1. Comparison of land cover classifications reported by the St. Joseph River Watershed Initiative (SJRWI) and those used in AnnAGNPS for the Cedar Creek Watershed.

| SWPI Classification | AnnAGNPS Classification | % of Total Land Area (SJRWI) | % of Total Land Area (AnnAGNPS) |
|---------------------|------------------------------------|------------------------------|---------------------------------|
| Cropland | Corn and Soybeans | 51 | 62.8 |
| CRP and Other | Pasture, CRP, Farmstead, and Other | 22 | 25.8 |
| Forest | Forest | 10 | 8.6 |
| Urban | Urban | 4 | 2.8 |
| Wetlands | Water | 13 | < 0.01 |
| Total | | 100 | 100 |

A description of land cover in the CCW and MDS was determined from the USDA National Agricultural Statistics Service (USDA-NASS, 2001), Indiana Cropland Data Layer. The approximate scale of the 2001 imagery used was 1:100,000 with a ground resolution of 30 by 30 m. The USDA-NASS (2001) Indiana Cropland Data Layer was converted from a raster file to an ESRI (Environmental Systems Research Institute, 1998) shapefile using ArcView. We evaluated the assigned land uses, and determined that there was an overestimation of pasturelands and farmsteads and underestimation of soybeans, corn, and forest. A manual correction was conducted by overlaying the intersected land use and cover shapefile (Int_lulc.shp) onto a color digital orthoquad (Purdue University, 2007) and the National Agricultural Statistics Service (USDA-NASS, 2001), Indiana Cropland Data Layer in Arcview, and reclassifying incorrectly assigned values. The corrected land cover was reasonably representative of the SJRWI-reported condition, as illustrated in Table 1 (SJRWI, 2005). For more detailed land classification maps, see Zuercher (2007).

Table 2. Corn planting progress with subsequent atrazine application in Indiana for 2006.

| Date | Cumulative Planted Area (%) | Incremental Change from Previous Application (%) | Atrazine Application (Kg/ha) (1.46 kg ha ⁻¹ * (%) incremental change) | Cumulative Rate(Kg/ha) |
|----------|-----------------------------|--|--|------------------------|
| April 17 | 3 | 3 | 0.04 | 0.04 |
| April 24 | 9 | 6 | 0.09 | 0.13 |
| May 1 | 33 | 24 | 0.35 | 0.48 |
| May 8 | 52 | 19 | 0.28 | 0.76 |
| May 15 | 74 | 22 | 0.32 | 1.08 |
| May 22 | 77 | 3 | 0.04 | 1.12 |
| May 30 | 89 | 12 | 0.18 | 1.30 |
| June 5 | 100 | 11 | 0.16 | 1.46 |

Management operations were assigned to each classification of land cover in the CCW and MDS. For agricultural data, area-specific information on management activities collected for CCW during February 2005 was used as input for the model. A corn and soybean crop rotation is predominate in both the CCW and MDS with the majority of planting occurring between late April and the end of May (USDA-NASS, 2006) with corn planting starting before soybeans. Atrazine is the primary herbicide utilized for weed control on corn acreage in the watershed, with the majority applied as a pre-emergent spray. Most soybeans (75%) in the CCW are genetically-altered to allow for weed control with the herbicide glyphosate (Larose, 2005). For this study, atrazine application was divided into eight applications with rates progressively increasing toward the peak corn planting time and then decreasing as the planting season tailed off. The number of atrazine applications was based on the number of crop reports available to determine planting progress during the corn planting season. The 2006 seasonal progress for corn planted in Indiana and the subsequent application rates can be found in Table 2. On average, the NASS Agricultural Chemical Database reported 1.01 atrazine applications per year for the 7-yr period from 1996 to 2002 with an average rate of 1.46 kg ha⁻¹ for Indiana (USDA-NASS, 2004).

DeKalb County, which contains the majority of the CCW and the entire MDS, had 28% of corn and 82% of soybeans in no-till systems during the 2004 crop year (Indiana Conservation Tillage Reports. 2004).

The total percentages of tillage practices in DeKalb County are located in Table 3 (Indiana Conservation Tillage Reports, 2004). AnnAGNPS determines land cover based on the dominant land cover for each cell; likewise, this study also utilized the dominant tillage practice for each crop cover. Due to the lack of accurate tillage practice spatial datasets and the fact that AnnAGNPS only utilizes the predominate management practice for each cell, this study utilized 100% conventional tillage practice for the corn rotation and 100% no-till for the soybean rotation.

Table 3. Percent tillage system reported in 2004 for DeKalb County, Indiana.

| County | Crop | Tillage System (%) | | | |
|--------|----------|--------------------|---------------|-----------------|----------------------|
| | | No-till | Mulch Tillage | Reduced Tillage | Conventional Tillage |
| DeKalb | Corn | 28 | 5 | 12 | 56 |
| | Soybeans | 82 | 3 | 3 | 11 |

This study utilized two crop and three non-crop management schedules. The two crop management schedules included a corn and soybean rotation and a continuous alfalfa management while the three non-crop management schedules were urban, fallow, and forest. The planting date was set to May 15 for corn and May 30 for soybeans. Harvest occurred on November 15 for the corn and October 15 for the soybeans. The alfalfa management consisted of a continuous cycle of hay re-growth and harvest with a fall senescence. The RUSLE database in the AnnAGNPS Input Editor was utilized to populate the annual root mass, cover ratio, rainfall height, and surface residue cover parameters in the non-crop section of the AnnAGNPS Input Editor. The RUSLE identifiers used in this study were forest, fallow, and residential, which was used for urban areas.

For simulation in the CCW, daily precipitation and maximum and minimum air temperatures were obtained from the NOAA National Climate Data Center (NOAA-NCDC, 2007) for the Garrett Station (Coop ID 123207) located at 41°20'N, 85°08' W elevation 265.2 m above sea level. This weather station is located within the CCW and contained the dataset from 1989 to 2006 required for the simulation periods of this study. Climate data for the MDS simulations was obtained from the USDA National Soil Erosion Research Laboratory (NSERL), Source Water Protection Initiative (SWPI) database for the time period of 2002-2006 at the sampling location AXL (41°24'58"N, 85°00'18"W). Other daily climate parameters were generated by processing the measured daily precipitation, and maximum and minimum air temperature data with the Complete_Climate program (USDA-ARS, 1999). A three-year period was used to initialize the soil moisture for the calibration and validation runs.

Table 4. Cedar Creek streamflow characteristics.

| USGS Station Name | Total Drainage Area (km ²) | Annual Mean Discharge Rate (m ³ s ⁻¹) | Annual Runoff (cm) | Annual Extreme Mean Discharge Rate (m ³ s ⁻¹) | | Baseflow (% of total runoff) |
|-----------------------------|--|--|--------------------|--|-----|------------------------------|
| | | | | Max | Min | |
| Cedar Creek near Cedarville | 699.3 | 7.2 | 32.6 | 13.7 | 2.4 | 48 |

The observed stream discharge data for the CCW was obtained from the U.S. Geological Survey (USGS) for the Cedar Creek gauge station 04180000 located near Cedarville, Indiana (41°13'08"N, 85°04'35"W) for January 1, 1989 to December 31, 2006. AnnAGNPS does not model subsurface flow, which means that stream discharge needs to be separated into its baseflow and direct runoff components. For this study, flow separation was done to achieve a baseflow percentage that matched the 48 percent baseflow reported by Beaty (1996). The daily stream discharge data was processed using the Eckhardt recursive digital filter method (Eckhardt, 2005) in the Web based Hydrograph Analysis Tool (WHAT) (Lim et al., 2005) with the filter parameter set to 0.980 and the Baseflow Index Maximum (BFI_{max}) set to 0.627. The processed daily stream discharge data had a baseflow index of 0.480 which corresponded well with the measured baseflow contribution in Table 4. The direct runoff portion of the daily stream discharge data was then averaged on a monthly basis to obtain results that would correspond to the monthly averaged output from AnnAGNPS.

Reliable observed stream discharge data for the MDS was available from April 1, 2006 to December 31, 2006 from the USDA NSERL SWPI database. This discharge data was collected using an ISCO 2150 AVF sensor with 2108 AD converter to ISCO 780 Analog module (Teledyne ISCO, 2007). Prior to 2006, only observed gauge height was available in the database; however, reliable flow discharge rating curves to convert stage to discharge have not yet been developed. Like Cedar Creek discharge, the Matson Ditch stream data was processed using the Eckhardt recursive digital filter method (Eckhardt, 2005) in the Web based Hydrograph Analysis Tool (WHAT) (Lim et al., 2005). Once baseflow separation was completed, the direct runoff portion of the daily stream discharge data was then averaged on a monthly basis to obtain results that would correspond to the monthly averaged output from AnnAGNPS.

The observed atrazine data for Matson Ditch was obtained from the USDA NSERL SWPI database for 2002-2006 at the AXL site. Like the stream discharge, atrazine data was only available for spring to fall, not continuously for a year, and it was averaged on a monthly basis.

Model Accuracy

The accuracy of AnnAGNPS simulation results was determined by examination of the mean, standard deviation (STDEV), coefficient of determination (R^2), the root mean square error (RMSE), and the Nash and Sutcliffe (1970) model efficiency coefficient (E_{NS}). A comparison of both mean and STDEV indicates whether the frequency distribution of model results is similar to the measured frequency distribution. The R^2 value is an indicator of the strength of the linear relationship between the observed and simulated values. The RMSE is indicative of the error associated with estimated streamflow. The E_{NS} simulation coefficient indicates how well the plot of observed versus simulated values fits the 1:1 line. The E_{NS} can range from $-\infty$ to +1, with 1 being a perfect agreement between the model and real data (Santhi et al., 2001). The simulation results were considered to be good if $E_{NS} \geq 0.75$, and satisfactory if $0.36 \leq E_{NS} \leq 0.75$ (Van Liew and Garbrecht, 2003). Negative values of model efficiency indicates that the mean of the observed data is a better predictor than the model (Van Liew and Garbrecht, 2003).

Calibration and Validation

Although all data sets were prepared using the AnnAGNPS version 3.57 a2 Arcview interface and input editor (Bingner and Theurer, 2005), the pollution loading model used in this study was version 4.00 a 023 (Bingner et al., 2007). Calibration of the AnnAGNPS model for stream discharge was done on a monthly basis for both the CCW and MDS. Model calibration was accomplished by comparing the baseflow separated observed stream discharge values and those produced from the AnnAGNPS simulations. The statistics for E_{NS} and R^2 were evaluated to determine the model's efficiency and the proportion of variation in observed discharge that is explained by the model output. Das et al. (2004) reported that the most sensitive AnnAGNPS parameters for runoff volume were the SCS runoff curve number (RCN) and precipitation and to a lesser degree the Manning's 'n' and hydraulic conductivity. For this study, calibration of stream discharge was accomplished by adjusting the RCN and interception evaporation values. Calibration simulations were performed until the E_{NS} and R^2 values exceeded 0.5 and further changes to corresponding calibration parameters failed to improve the model's performance. Calibration period for the CCW flow was from January 1989 – December 1998, while the validation period was from January 1999 – December 2006. For the MDS, reliable flow data was only available for April-December 2006, so only calibration was possible.

Atrazine concentration calibration for MDS was conducted after the hydrology had been calibrated. Since there were no previous calibration studies for pesticides using the AnnAGNPS model, there was no information on the sensitivity of the model for any of the pesticide parameters. For this study, pesticide calibration was achieved by adjusting the percentage of pesticides applied to the soil and foliage and percentage washoff from foliage. These parameters were chosen because they did not interfere with the stream discharge calibration and tended to be variable under different management and field conditions. Like the stream discharge calibrations, calibration of pesticide concentrations was completed when E_{NS} and R^2 values exceeded 0.5 and further changes to corresponding calibration parameters failed to improve the model's performance. Atrazine calibration period was April-December 2006, while validation period was June 2002 – October 2005.

Results and Discussion

Initial AnnAGNPS simulation results for the CCW, prior to calibration are shown in Table 5 and Figure 2a. Examination of the evaluation statistics for stream discharge predictions showed satisfactory performance. The results indicated that the mean stream discharge was overestimated by about 26% and the time series data shown in Figure 3 showed a consistent overprediction in the months of July through January.

Table 5. Cedar Creek Watershed monthly stream discharge prior to calibration.

| Time Period | Mean ($\text{m}^3 \text{s}^{-1}$) | | St. Dev. ($\text{m}^3 \text{s}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|-------------------------------------|----------|---|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 1989-1998 | 5.34 a | 4.24 a | 5.98 | 4.61 | 0.44 | 0.71 | 3.34 |

* Means followed by the same letter are not significantly different in a simple t-test with $\alpha=0.05$.

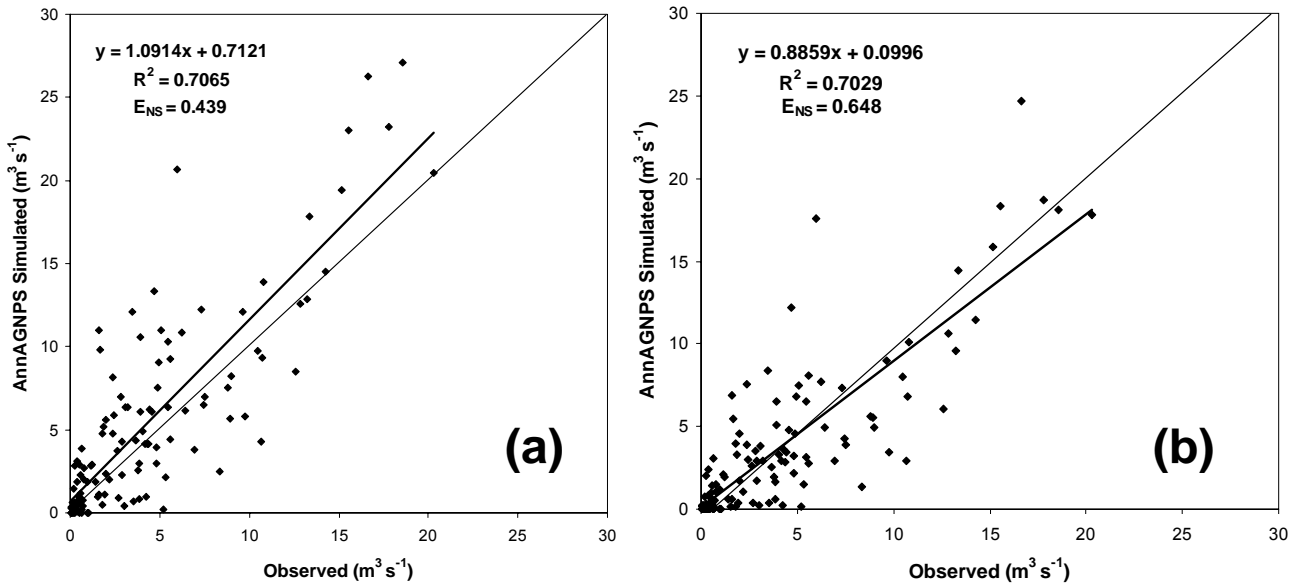


Figure 2. Simulated versus observed stream discharge a) before calibration and b) after calibration for Cedar Creek Watershed.

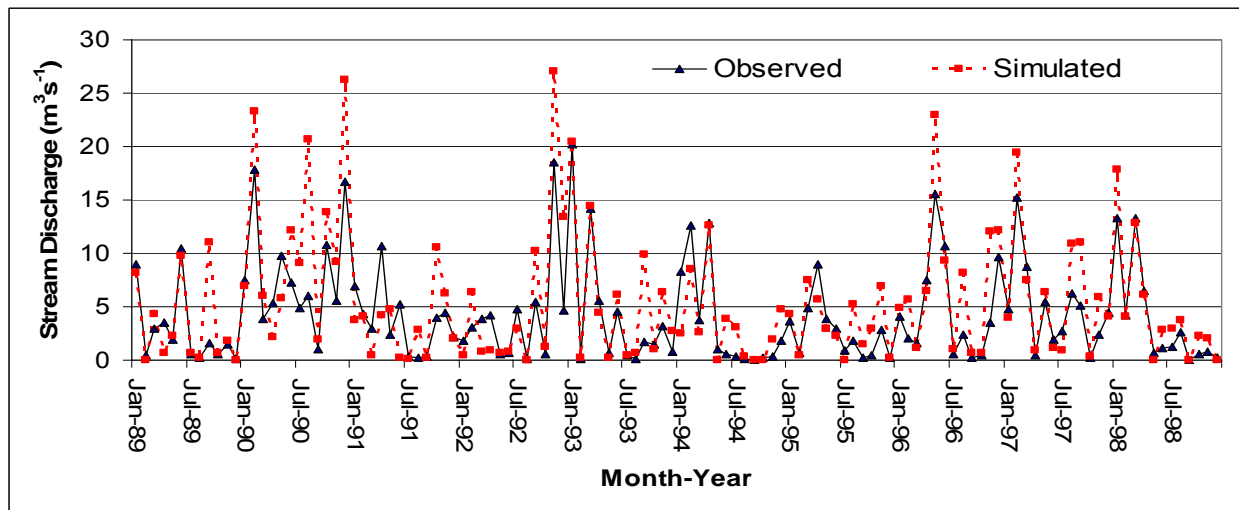


Figure 3. Observed and simulated monthly stream discharge versus time before calibration for the Cedar Creek Watershed.

Cedar Creek Flow Calibration and Validation

Calibration of stream discharge in CCW was conducted on a monthly basis for January 1, 1989 to December 31, 1998. The initial model simulations found that stream discharge was overpredicted. Thus, RCN values for agricultural land were decreased by 10% and the model re-run. Results showed that a 10% reduction in RCN was not sufficient to reduce runoff to the observed level and also indicated that the default maximum and minimum rainfall interception values were likely too low. Bingner (personal communication May 2007) had similar problems with AnnAGNPS modeling of the Auglaize River Watershed in northwest Ohio.

At this point, RCN values for agricultural land were returned to the initial values and the maximum and minimum interception evaporation values were increased. This process of increasing maximum and minimum interception evaporation values continued until the observed and predicted stream discharge values were nearly equal. The final value for minimum rainfall interception used in this study was 1.99 mm and the maximum interception evaporation value was 5.08 mm. Although much higher than the default values of maximum (2.5 mm) and minimum (0.2 mm), the minimum is within the range of value observed by Savabi and Stott (1994) for various crop residues and the maximum is well within the average value of 12.3 mm reported by Brye et al. (2000) for prairie residue. Savabi and Stott (1994) reported average rainfall interception values of 2.3, 2.0, and 1.8 mm for winter wheat, soybeans, and corn residue, respectively. The adoption of conservation tillage, which increases residue, the implementation of CRP, and 10% forest in the CCW likely explain these elevated values. After modifying these interception values, RCN for agricultural land required additional adjustments. This time when they were increased by 10 percent it resulted in an appreciable increase in prediction accuracy. However, stream discharge values for spring were overestimated, so early spring RCN values for agricultural land were returned to their original levels. Calibration of the model for stream discharge for the CCW was now considered to be complete.

Post calibration simulations in the CCW showed significant improvement in the E_{NS} and mean discharge values. Resulting mean discharge was 10% less than the predicted value, a 16% improvement compared to the uncalibrated model. The E_{NS} , as illustrated in Table 6 and Figure 2b, was 0.21 greater than the uncalibrated model, indicating that the calibrated model was a much better predictor of the observed stream discharge values. The time series data appears much more reasonable with far fewer overpredictions, minimal underpredictions and greater accuracy during the July to January time period (Figure 4).

Table 6. Cedar Creek Watershed monthly stream discharge statistics after calibration.

| Time Period | Mean (m^3s^{-1}) | | St. Dev. (m^3s^{-1}) | | E_{NS} | R^2 | RMSE |
|-------------|----------------------|----------|--------------------------|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 1989 - 1998 | 3.86 a | 4.24 a | 4.87 | 4.61 | 0.65 | 0.70 | 2.72 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

The major improvements in the summer months of July through September can be attributed to the increase in the maximum and minimum rainfall interception utilized during calibration. Since AnnAGNPS assumes that the actual evaporation on any given day's precipitation varies linearly between the maximum and minimum interception rates as a function of humidity (Bingner and Theurer, 2005), it is likely that the summer and fall months, with their higher average daily humidity, drastically limited interception evaporation when the default value was used.

Validation results from the calibrated model were satisfactory (Table 7 and Figures 5-6). The statistics were not as good as those obtained in the calibration period (E_{NS} reduced by 0.19 and R^2 reduced by 0.10), though this is to be expected. As illustrated in Figure 6, the trend for simulated values was lower than the observed values. This relationship was nearly identical to that observed in Figure 2b of the calibrated data. As was the case with the calibrated data, the values from January to June contained the majority of the underestimated values and those from July to December approached or exceeded the observed (Figure 5). This trend was likely associated with humidity, plant growth and seasonal patterns in the rainfall.

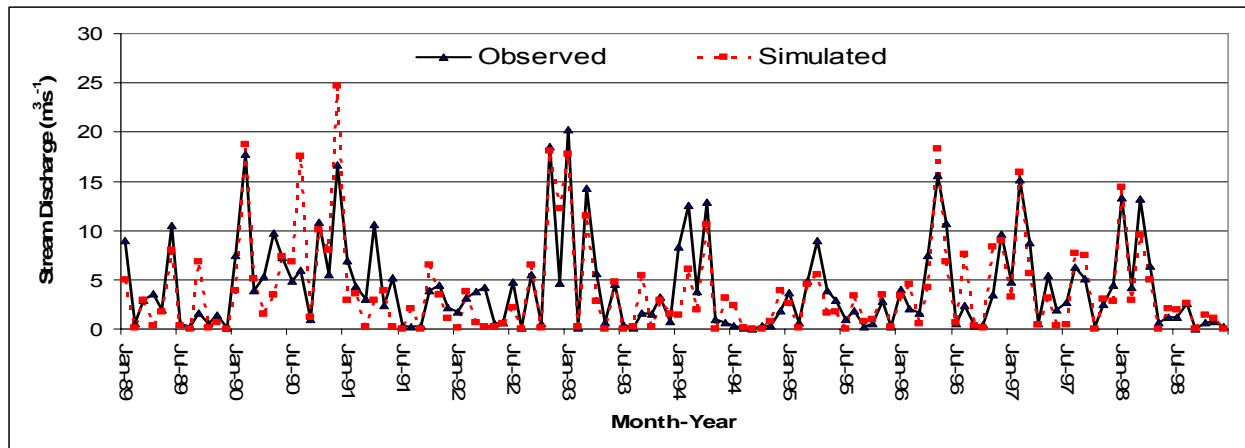


Figure 4. Observed and simulated monthly stream discharge versus time after calibration for Cedar Creek Watershed.

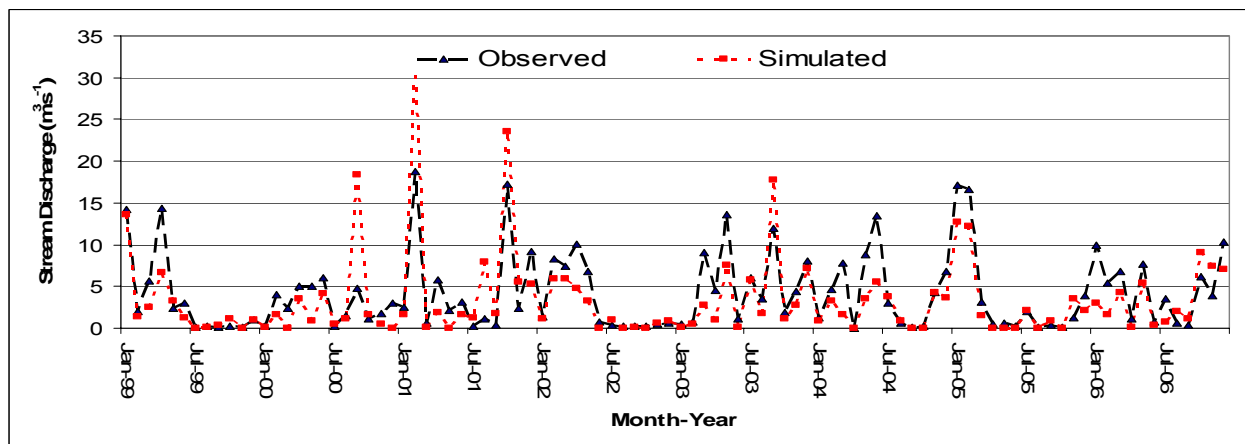


Figure 5. Observed and simulated monthly stream discharge versus time during validation period for the Cedar Creek Watershed.

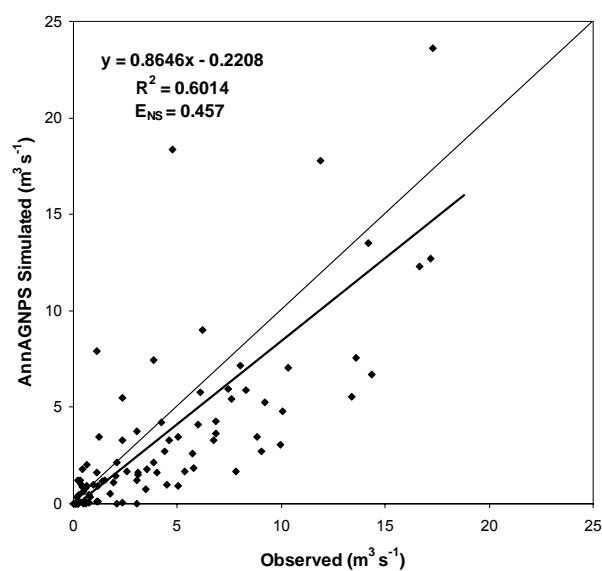


Figure 6. Simulated versus observed stream discharge for validation period for Cedar Creek Watershed.

Table 7. Cedar Creek Watershed monthly stream discharge validation statistics.

| Time Period | Mean ($\text{m}^3 \text{s}^{-1}$) | | St. Dev. ($\text{m}^3 \text{s}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|-------------------------------------|----------|---|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 1999-2006 | 3.63 a | 4.15 a | 5.15 | 4.62 | 0.46 | 0.60 | 3.38 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

Calibration of atrazine concentrations for the CCW was not conducted for this study as the available USGS NAWQA (National Water-Quality Assessment Program) observed data was in the form of grab samples that were taken approximately once every week and did not sufficiently capture monthly variations in pesticide concentrations. Future studies with more detailed NSERL monitoring data will allow model evaluations for pesticides at this larger scale.

Matson Ditch Flow Calibration

Calibration of the model in the MDS involved two stages, one stage for stream discharge and the other for pesticide concentrations. Stream discharge and atrazine concentration calibrations were performed on a monthly basis for the period of April 1, 2006 to December 31, 2006 in the MDS. The one year calibration period was selected as it was the only time period when both atrazine concentrations and stream discharge data were directly measured. Utilization of a short calibration period likely limited the model's precision as it was not possible to select parameter values that could be calibrated over a wider range of climatic variation.

Similarly to CCW, the calibration for Matson Ditch involved first adjusting the rainfall interception evaporation values and secondly adjusting the RCN for agricultural land. Initial results indicated that the model overpredicted stream discharge. Subsequently, the final rainfall interception minimum and maximum were reduced to 0.0508 mm and 1.016 mm respectively. The reduced rainfall interception values in the MDS were likely due to the lack of CRP and forest; as neither make up one percent of the predominant land cover identified in the model and both have high rainfall interception rates (Gash et al., 1995; Clark, 1940). At this point, the RCN values were adjusted to increase the model's performance. Like the CCW, the MDS illustrated the same systematic differences in agricultural land RCN values with a 10% increase throughout the late spring to the end of end of winter and 10% decrease in early spring.

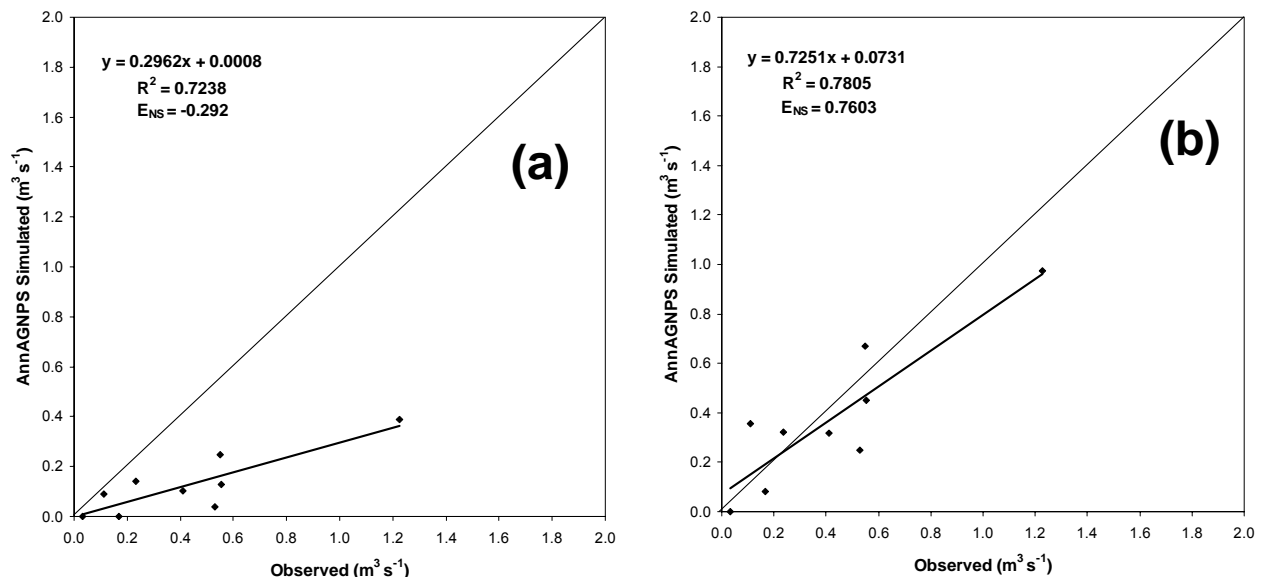


Figure 7. Simulated versus observed stream discharge a) before calibration and b) after calibration for the Matson Ditch Subwatershed.

Calibration of the MDS was only completed for a nine month time period from April 2006 to December 2006. Due to limited amount of accurate stream discharge data for MDS, this short time period of data was the only workable option. Prior to calibration, results for MDS were unacceptable with significantly

different observed and simulated mean stream discharges as shown in Table 8. In addition, the negative E_{NS} value (-0.29) indicated that the model was not an adequate predictor of the observed values. The linear regression line indicated that the overall model trend for simulated values was drastically below the observed values (Figure 7a). The time series data in Figure 8 shows that the simulated stream discharge had peaks and recessions in the same months as the measured, but magnitudes were greatly underestimated, and the differences in simulated and observed values grew as stream discharge increased. This trend was likely due to an overestimation of infiltration and rainfall interception.

Table 8. Matson Ditch monthly stream discharge statistics before calibration.

| Time Period | *Mean (m^3s^{-1}) | | St. Dev. (m^3s^{-1}) | | E_{NS} | R^2 | RMSE |
|-------------|-------------------------------------|----------|--|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 2006 | 0.13 b | 0.42 a | 0.13 | 0.36 | -0.29 | 0.72 | 0.39 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

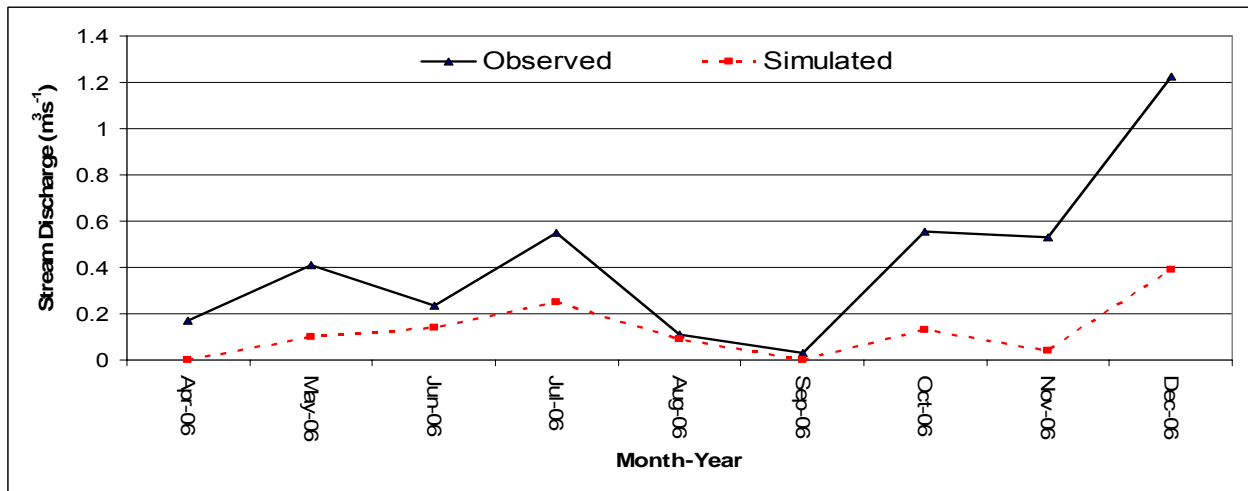


Figure 8. Observed and simulated monthly stream discharge versus time before calibration for Matson Ditch Sub-catchment.

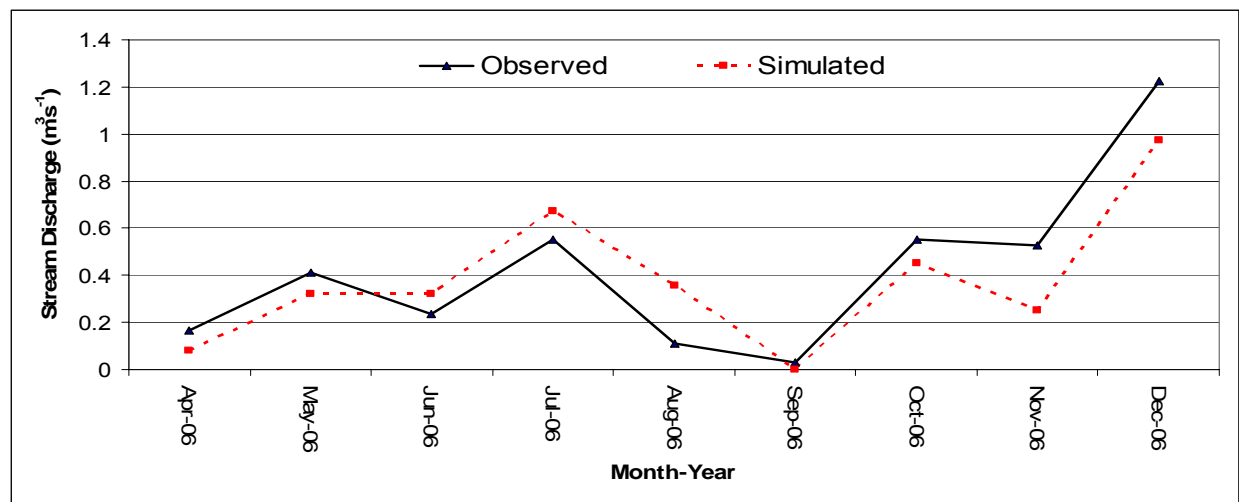


Figure 9. Observed and simulated monthly stream discharge versus time after calibration for Matson Ditch Sub-catchment.

After calibration, the model statistical results greatly improved, with the E_{NS} increasing to 0.76 and R^2 increasing to 0.78, and the mean stream discharge values were no longer significantly different (Table 9). The linear regression equation in Figure 7b illustrated that observed values were still underestimated but the extent to which this occurred was much more limited. Additionally, Figure 7b shows that the model

overpredicted when the observed monthly average discharges were below $0.3 \text{ m}^3 \text{ s}^{-1}$ and underpredicted when they were above $0.3 \text{ m}^3 \text{ s}^{-1}$. The time series stream discharge data (Figure 9) demonstrated that the model overpredicted from June through August. Since this time period corresponds with increased crop cover, this pattern was likely related to the crop cover's interaction with precipitation. It is possible that the interception, evapotranspiration, and plant uptake were underestimated during this time period and overestimated from post harvest to crop emergence. Interception evaporation likely played the largest role since it was reduced during calibration to obtain better model performance. As AnnAGNPS only allowed single maximum and minimum values throughout the entire simulation, it is likely that the calibrated value was actually below the true value during the crop growing season and above the true value when the field cover was reduced. Although this discrepancy existed, the model's hydrologic performance for MDS was classified as satisfactory based upon the overall statistical results.

Table 9. Matson Ditch monthly stream discharge calibration statistics.

| Time Period | *Mean ($\text{m}^3 \text{ s}^{-1}$) | | St. Dev. ($\text{m}^3 \text{ s}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|---------------------------------------|----------|--|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 2006 | 0.38 a | 0.42 a | 0.30 | 0.36 | 0.76 | 0.78 | 0.17 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

Matson Ditch Atrazine Calibration & Validation

Calibration of atrazine concentrations was conducted for the time period of April 1, 2006 through October 31, 2006 as these were the only complete months of observed pesticide and stream flow data. Atrazine concentration calibration was achieved by adjusting the percentage of pesticides applied to the soil and foliage and percentage of pesticide washoff from foliage.

After the initial run of the calibrated to stream discharge model, pesticide concentrations were unrealistically low (Figure 10). After exhaustively evaluating the inputs to the model with no improvement, concern was raised that the model pesticide routine was not functioning properly.

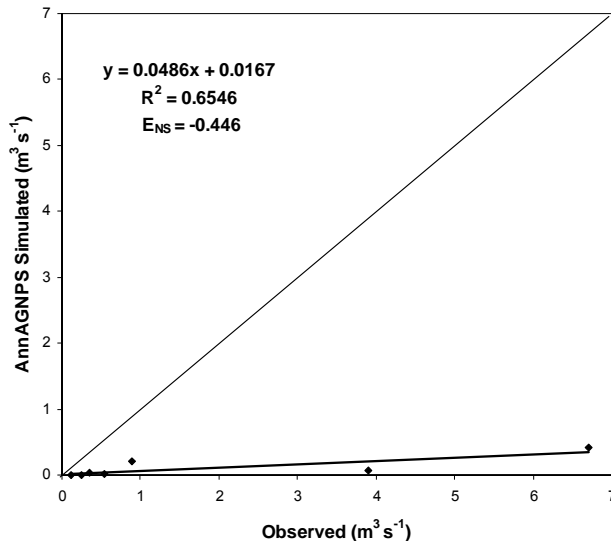


Figure 10. Simulated versus observed stream discharge for Matson Ditch Sub-catchment prior to code corrections.

Correction to AnnAGNPS model code

A copy of the AnnAGNPS PL model version 4.00 a 023 source Fortran code was obtained from the model developers and analyzed for errors. Testing and evaluation revealed an error in line 1035 of Insitu_Routines/Insitu_Pesticides.f90. The original line read: $\text{rnof_H2O} = \text{cell_sur_rnof} / \text{ptcs\%da_tot}$, where cell_sur_rnof is defined as surface unit area flow (mm), ptcs\%da_tot is total drainage area of the

cell (ha), and **rnof_H2O** is cell runoff (cm). The GLEAMS code in the model expects runoff to be in centimeters. To obtain this, the value for cell surface runoff needs to be in megagrams. In the corrected code this is now calculated and given the value **cell_sur_rnof_Mg**. The corrected GLEAMS code sequence in AnnAGNPS now reads:

```
IF (ptcs%da_tot > 0.) THEN
    rnof_H2O = cell_sur_rnof_Mg / ptcs%da_tot ELSE
    rnof_H2O = 0.
ENDIF
rnof_H2O = rnof_H2O / 100
```

Due to this error, input runoff depth for the pesticide calculations was drastically underestimated, helping to explain the original unrealistically low pesticide output values. This error and correction was reported to the AnnAGNPS model developers, and their response was that the evaluation was correct and an updated version of AnnAGNPS with this correction would be publicly released in the near future (R. Bingner, personal communication, 10/24/2007).

Additionally, the AnnAGNPS Version 2: User Documentation (Bingner and Theurer, 2001) which explains the model output has the upstream and downstream event attached and dissolved pesticides reversed. The event attached and dissolved pesticides downstream are actually on line 18 fields 7 and 8, respectively, and the upstream are on line 17 fields 7 and 8, respectively.

Simulations were re-run with the corrected model code, and the initial uncalibrated pesticide predictions were now much greater than those observed (Table 10).

Table 10. Matson Ditch monthly atrazine concentration statistics before calibration with corrected code.

| Time Period | *Mean ($\mu\text{g l}^{-1}$) | | St. Dev. ($\mu\text{g l}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|--------------------------------|----------|-----------------------------------|----------|----------|-------|--------|
| | Simulated | Observed | Simulated | Observed | | | |
| 2006 | 63.30 b | 1.91 a | 88.35 | 2.77 | -1538.6 | 0.33 | 100.66 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

The initial model output from the corrected model drastically overestimated the observed values. As shown in Table 10, the mean simulated value was approximately 33 times larger than the observed and the E_{NS} value was very negative. The model greatly overpredicted pesticide concentrations at application and moved nearer to the observed in September.

As a result, it was determined that more of the atrazine needed to be applied to foliage since crop residue can act as foliage in AnnAGNPS (R. Bingner, personal communication, May 2007). Additional simulations confirmed that the model overpredicted when as little as five percent of the atrazine was soil applied. As a result, additional calibration runs proceeded with 100% of the atrazine applied to the foliage.

Final calibration of the model was accomplished with 100% of the atrazine applied to the foliage and the pesticide washoff fraction adjusted to 14%, from 45%. The statistical results (Table 11) indicated that the calibrated model had good performance in predicting atrazine concentrations for the very limited 7 month period studied here. The linear regression line in Figure 11 was consistently near the 1 to 1 line meaning that there was limited over- or under- prediction of the model. With the exception of the month of July, the time series data (Figure 12) exhibited exceptional consistency, which revealed AnnAGNPS's ability to accurately predict atrazine degradation timing when the model was appropriately calibrated.

Table 12. Matson Ditch monthly atrazine concentration calibration statistics.

| Time Period | *Mean ($\mu\text{g l}^{-1}$) | | St. Dev. ($\mu\text{g l}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|--------------------------------|----------|-----------------------------------|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 2006 | 2.04 a | 1.91 a | 2.69 | 2.77 | 0.93 | 0.93 | 0.69 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

Although this calibration of the model showed good results, it is not really correct to apply 100% of the atrazine to the foliage. In addition, the percentage of attached pesticides was drastically overestimated in the model output. The calibrated pesticide model output showed roughly 12,000 times more attached than dissolved pesticide. Since atrazine is moderately soluble (33 mg L^{-1}), the concentration of dissolved pesticide should greatly exceed the sediment attached fraction. The Mickleson et al. (2001) study of various tillage and incorporation techniques for pesticides near Boone, Iowa reported that at least 95% of the total loss of atrazine recorded in the study was found in solution.

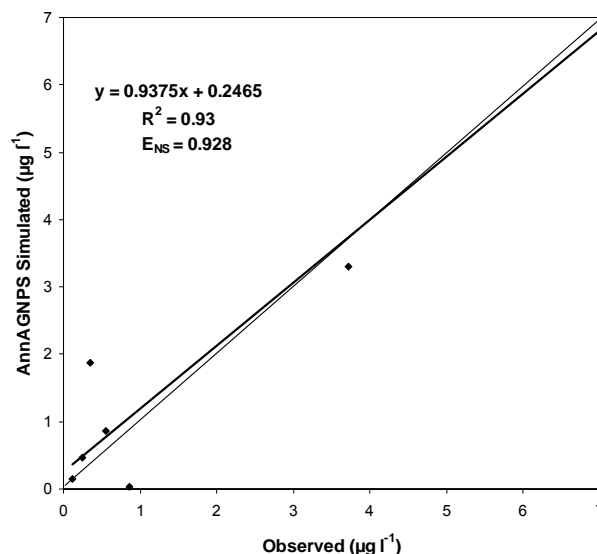


Figure 11. Simulated versus observed atrazine concentration for 2006 after calibration for Matson Ditch Sub-catchment.

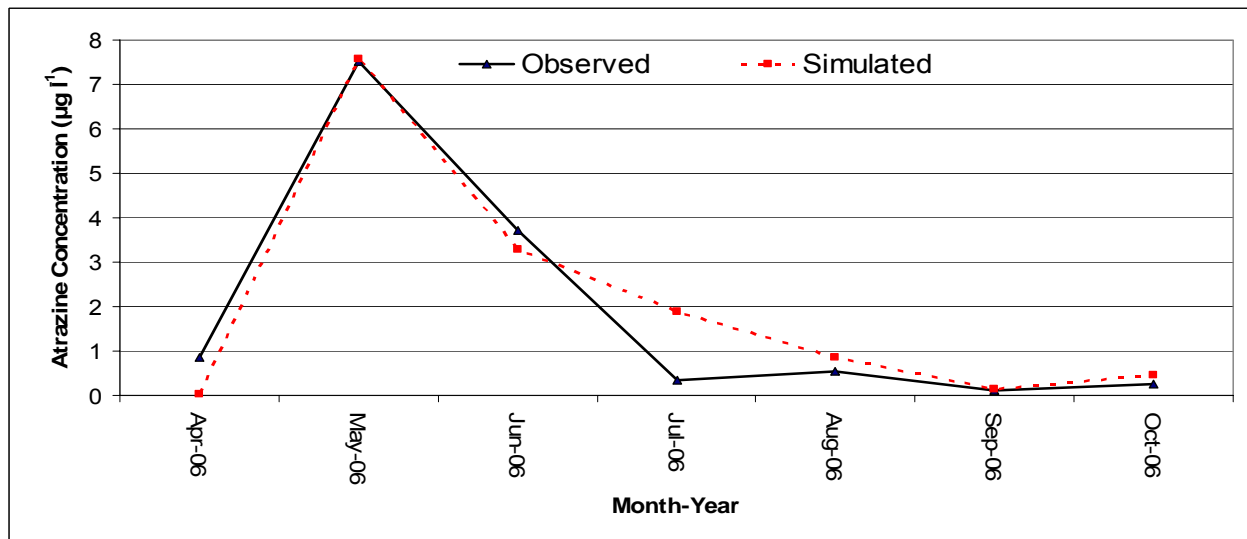


Figure 12. Observed and simulated monthly atrazine concentration versus time after calibration for Matson Ditch Sub-catchment in 2006.

Validation for monthly values during 2002-2005 with the corrected and calibrated AnnAGNPS model showed very good results with an E_{NS} of 0.82 and R^2 of 0.88, as shown in Table 13. This is quite encouraging given the extremely limited calibration period used here. The linear regression line on the 1 to 1 plot in Figure 13 falls below the 1 to 1 line which indicates that the model has an overall tendency to underpredict atrazine concentrations. The graph of time series data in Figure 14 showed that simulated atrazine concentrations exhibited only slight seasonally consistent deviations from the observed concentrations. The consistent deviations occurred during the months of June and July where the model

underpredicted for three of the four years. The lack of seasonal inconsistencies demonstrates the applicability of the calibrated model over a wide range of climactic and crop growth conditions.

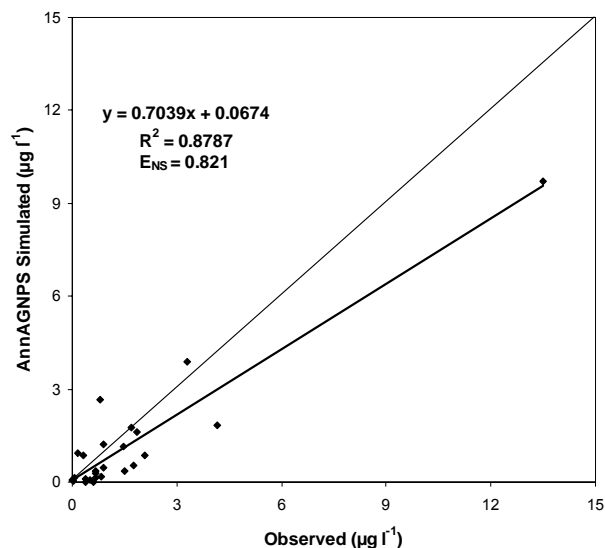


Figure 13. Simulated versus observed atrazine concentration for validation period for Matson Ditch Sub-catchment.

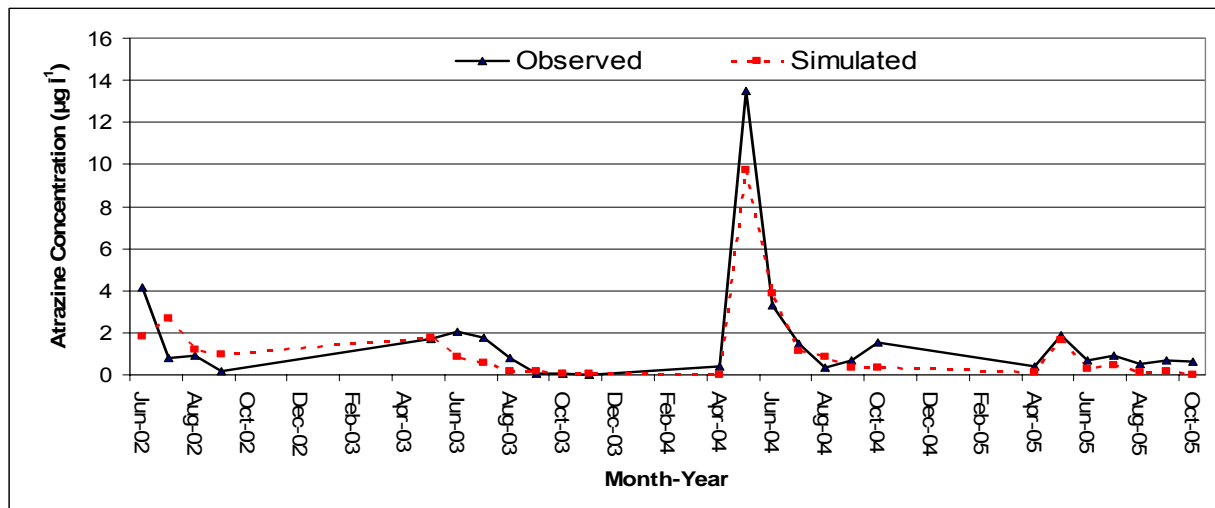


Figure 14. Observed and simulated monthly atrazine concentration versus time for the validation period for Matson Ditch Sub-catchment.

Table 13. Matson Ditch monthly atrazine concentration validation statistics.

| Time Period | *Mean ($\mu\text{g l}^{-1}$) | | St. Dev. ($\mu\text{g l}^{-1}$) | | E_{NS} | R^2 | RMSE |
|-------------|--------------------------------|----------|-----------------------------------|----------|----------|-------|------|
| | Simulated | Observed | Simulated | Observed | | | |
| 2002 -2005 | 1.17 a | 1.57 a | 2.01 | 2.68 | 0.82 | 0.88 | 1.11 |

* Means followed by the same letter are not significantly different in simple t-test with $\alpha=0.05$.

Summary and Conclusions

The AnnAGNPS model hydrologic and pesticide routines were evaluated for their effectiveness at predicting stream discharge in the 707 km² CCW and the 45 km² MDS, and atrazine concentrations in runoff water in the MDS. A USGS 1/3 arc-second DEM that was resampled to an exact 10 meter grid and

burned in one meter with the stream networks from NHD was used to delineate the CCW into 942 cells that averaged 75 ha in size. Spatial soil data for both watersheds was obtained from SSURGO while the physical soil properties originated from the National Soil Information System (NASIS) soil database. Dominant land use was determined by intersecting the delineated cells with the converted shapefile from the USDA NASS Indiana Cropland Data Layer. Management inputs such as the type of crops grown, tillage practices, fertilizers and pesticides used and the dates when field operations occurred came from the St. Joseph River Watershed Initiative (SJRWI) project, and the Soil and Water Conservation Districts (SWCD) of Allen, DeKalb, and Noble Counties.

The model was calibrated and validated against the best available data for each watershed. Hydrologic calibration simulations were performed from 1989 through 1996 for the CCW, with a resulting E_{NS} of 0.65, and in 2006 for the MDS which resulted in an E_{NS} of 0.76. These results indicated that the model could be satisfactorily calibrated to both the MDS and CCW. Validation of the model calibrated to the CCW was done using independent data from 1997 until 2006 with a resulting E_{NS} of 0.46. Insufficient flow data were available for validation in the MDS. The satisfactory statistical results and evaluations of the flow time series graphs indicated that model runoff predictions were reasonable.

Initial simulations for atrazine pesticide losses led to examination of the model source code, and ultimately correction of an error that had caused major underpredictions of atrazine losses. The original AnnAGNPS source code mistakenly routed runoff into the pesticide code as depth of runoff, not the mass that the routine expected. Corrections were made to the AnnAGNPS source code to properly route the runoff mass into the pesticide routine, and the corrected code was used for pesticide simulations in the MDS for 2002 through 2006. The results showed that calibration of the model to the MDS could produce very good results with an E_{NS} of 0.93. However, calibration and validation for atrazine concentration was only possible by applying 100 percent of the atrazine to foliage, which is not realistic. Validation of the model was conducted from 2002 through 2005 and the resulting E_{NS} of 0.82 indicated that the model was capable of producing very satisfactory predictions of atrazine concentrations in runoff in the MDS. Calibration and validation of the pesticide routine was not conducted in the CCW as there was a lack of adequately measured pesticide data.

Overall, this study found that the calibrated AnnAGNPS model produced satisfactory validation results for stream discharge. It also revealed a number of problems within the pesticide routine of AnnAGNPS and showed that predictions of atrazine concentrations could be successfully calibrated with the corrected model.

Further review of the AnnAGNPS pesticide routine is needed to determine the cause of the underprediction of atrazine in solution, and overprediction of total atrazine runoff when atrazine is soil applied. Additionally, a sensitivity analysis is needed to determine why the model was relatively insensitive to RCN adjustments and quite sensitive to maximum and minimum interception evaporation adjustments. Future research needs to attempt calibration of the model to the NAWQA data for the CCW, since data collected using a weekly grab sample approach is more widely available than daily sampling.

Acknowledgements

The authors would like to acknowledge Dr. Ronald Bingner for his substantial assistance on AnnAGNPS setup and application. Mr. Jim Frankenberger provided enormous help in debugging and correcting the AnnAGNPS model code. The late Mr. Charles Meyer contributed in development of software to read and display relevant model outputs for this research.

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